Topological Feature Extraction for Quantitative Analysis of Terascale Combustion Simulation Data

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Summary

One of the major challenges in improving modern energy production methods is to reveal the key chemical processes that underlie the complex mechanisms of combustion. This has motivated the development of advanced computational methods aimed at the Direct Numerical Simulation of the full three-dimensional dynamics of turbulent flames. Better analyzing and understanding the details of such flames will enable new insights into reducing pollutants and increasing efficiency in combustion devices. The objective of this collaborative research is twofold: first, to develop a method to characterize the mixing length scales in a turbulent flow simulation on an instantaneous and local basis; second, to explore the interaction between mixing and autoignition. These goals are accomplished via a new family of roust combinatorial methods that we use to identify, segment and track in time topological features related to local mixing rates and to a scalar representative of autoignition. This research could have long-term impact in a number of application areas related to energy production such areas as in jet aircraft engines, where fuel and oxidizers are not premixed for safety reasons, and in direct-injection internal combustion engines where diesel jet flames are stabilized downstream of the fuel injector in a hot ignitive coflow.

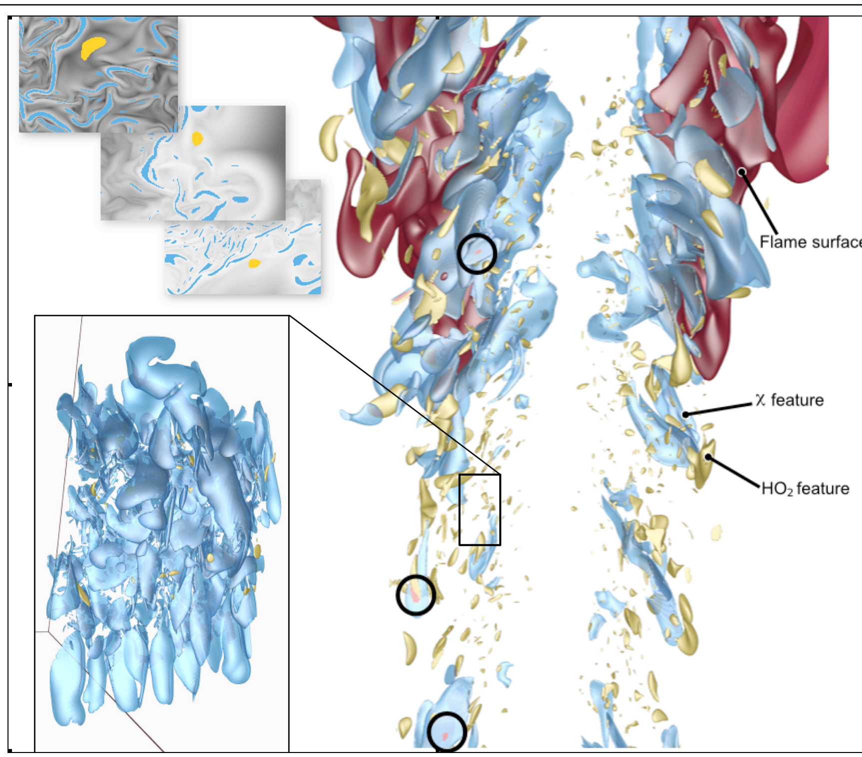
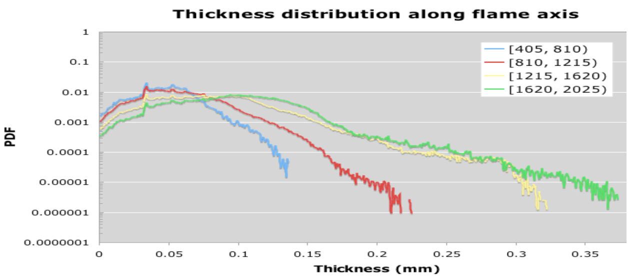
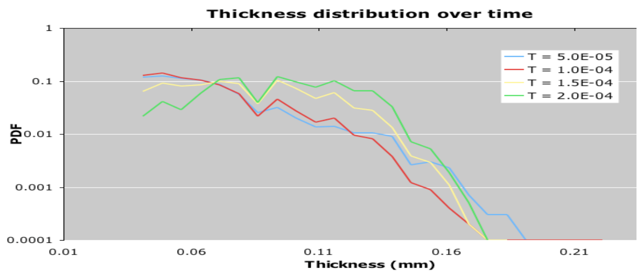


Figure 1. Topological analysis of a combustion simulation. Maxima of HO2 species (gold) can indicate auto-ignition kernels. These kernels are expected to live outside high-χ regions (blue regions). High-χ regions are large and many compared to HO_2 regions. Right, all HO2 kernels below the base of the flame with high-χ segments that overlap them. Bottom-left, close-up side view showing all HO2 kernels and high-χ segments. Top-left, three cross sections showing the relation between the HO2 and χ fields.





In turbulent non-premixed combustion, where the fuel and oxidizer reactant streams are segregated, the reactant streams must be molecularly mixed before reaction can occur. Therefore, the turbulent mixing rate is a key quantity in determining the overall burning rate and efficiency. In general, as the mixing rate increases, reaction rates increase and the overall efficiency increases. A nonpremixed flame has a well-defined internal structure. Beyond a critical rate of mixing reactions cannot keep up with the mixing and the flame quenches locally. This undesirable situation can lead to increased emissions. If quenching is pervasive, then global blow-out can occur, which would be catastrophic, for example, in an aero gas-turbine engine. In an autoignition situation, there is a similarly well-structured relationship between the species concentrations but the relationship is in time instead of space as radical concentrations build up to sufficient levels to establish a flame. Turbulent mixing is characterized locally by the scalar dissipation rate, χ, which is equal to twice the product of the molecular diffusivity and the square of the mixture fraction gradients.

3D measurements have shown that the thickness of χ scales not with the integral scale of turbulence, but rather, with the small-scale turbulence, i.e. the Kolmogorov or Batchelor scales. The advent of terascale 3D direct numerical simulations (DNS) of moderate Reynolds number turbulent reactive jet flames has enabled the direct computation of χ and its evolution. For the purpose of characterizing the regime of the simulation, we no longer need to estimate local mixing dimensions from the large-scale expected values of the turbulence field, as we have the scalar dissipation rate field itself available. The method presented here is devised to use the resolved χ field to identify and measure the structure of extinction and autoignition regions. We study the results from two DNS simulations. The First is a temporally-evolving turbulent CO/H2 jet flame undergoing extinction and reignition at different Reynolds numbers (left of Figure 2). The second is a spatially-evolving lifted turbulent Ethylene/air jet flame. This simulation, performed on a grid of 1 billion grid points, is depicted on the right of Figure 2. In this arrangement, the configuration is statistically stationary in time.

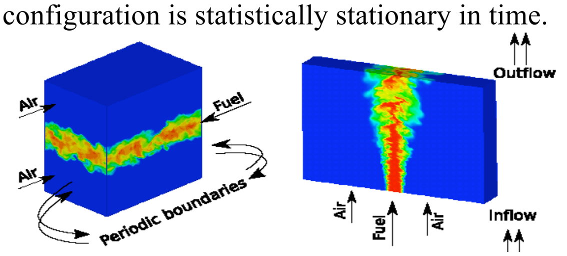


Figure 2. Schematic of combustion scenarios. Left, the temporally evolving jet. Right, the lifted jet.

With our topological approach we are able to provide robust segmentation and tracking of high-χ regions (Fig.1). This allows for the first time to perform a quantitative analysis of the thickness of these features and their distribution in space and time. These statistics are shown the top for both the lifted jet case (on the left) and for the dynamic case (on the right). Our method is capable of determining a highly localized measure of the mixing length and shed new insight in the detailed dynamics of extinction and reignition processes. Application to terascale data sets indicates that the method can be applied to very large datasets on modest hardware. This is a particularly useful since the hardware used for the original simulation is out of reach for most of the combustion community and, using higher end resources, gets are closes to the petascale data analytics regime.

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